Decision Trees

Decision Trees

Split data along feature data range, typically binary decisions

- Scalar: find delimiter
- Discrete: yes/no



Regression example





Heinen et al, J Chem Phys, 2021.

When to use

Pros

- Easy to interpret / visualize
- Cheap to use
- No data standardization necessary
- Works well with large amounts of training data (need exponentially more data for another level)
- Flexible: both regression and classification

Cons

- Costly to train
- Prone to overfitting
- Overfitting in high dimensions
- Struggles with "diagonal data"
- Struggles with imbalanced data sets
- Instable under changed of training / randomization Consider random forests

- How to fix
- Consider random forests
- Restrict depth of tree
- Subselect features
- Transform features with principal components
- Subsample

How to build a tree?

Finding the minimal tree is costly.

Heuristic

- Choose feature
- Choose delimiter
- Repeat



Node splitting

A good tree is

- Small
- Important decisions at the root

Typically: maximise information gain from entropy

$$IG(T, A) \equiv H(T) - H(T|A)$$
Information entropy Conditional entropy

$$H(T) \equiv -\sum_{\substack{t \in \mathcal{T} \\ \text{Probability} \\ \text{Possible values}}} p(t) \log p(t) \qquad H(T|A) \equiv -\sum_{\substack{a \in \mathcal{A}, t \in \mathcal{T} \\ \text{Probability} \\ \text{Probabili$$

1)

Information gain example

Two fair dice, looking for the sum. Which one if rolled first tells us more?

$$Q\equiv D_1+D_2$$
 D_1 0 1 D_2 0 1 2

$$H(T) \equiv -\sum_{t \in \mathcal{T}} p(t) \log p(t)$$

$$\begin{array}{ccccc} \mathsf{D}_{1} & \mathsf{D}_{2} & \mathsf{Q} \\ 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 2 & 2 \\ 1 & 0 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 3 \end{array} \quad H(D_{1}) = -\log_{2}\frac{1}{2} = 1 \\ H(D_{2}) = -\log_{2}\frac{1}{3} \simeq 1.585 \end{array}$$

Information gain example

 $Q\equiv D_1+D_2$ D_1 o 1 D_2 o 1 2

$$H(T|A) \equiv -\sum_{a \in \mathcal{A}, t \in \mathcal{T}} p(a, t) \log \frac{p(a, t)}{p(a)}$$

Q/D₁ 0 1 2 3
0 1 1 1 1
$$H(Q|D_1) = -6 \cdot \frac{1}{6} \log_2 \frac{1/6}{1/2} \simeq 1.585$$

1 1 1 1

Q/D₂ 0 1 2 3 0 1 1 1 1 $H(Q|D_2) = -6 \cdot \frac{1}{6} \log_2 \frac{1/6}{1/3} = 1$ 2 1 1 1

Information gain example

$$Q\equiv D_1+D_2$$
 D_1 o 1 D_2 o 1 2

 $IG(T,A) \equiv H(T) - H(T|A)$

 $IG(Q, D_1) = \frac{1}{3}$



Choose the second dice first yields the higher information gain.

Node splitting

Maximize information gain from entropy

 $IG(T, A) \equiv H(T) - H(T|A)$

- H(T|A)=H(T) if A and T uncorrelated, then IG(T, A) = 0
- Adding or removing unused values t has no effect on H

$$H(T) \equiv -\sum_{t \in \mathcal{T}} p(t) \log p(t)$$
Probability
Possible values

Fixing overfitting

Pruning

- More data
- Simpler trees
 - Restrict during construction (depth, number of data points per leaf)
 - Remove least degrading nodes afterwards

Random forests

- Have many randomized decision trees
- Take majority vote
- An example of an ensemble method

Summary Decision Trees

- Idea: Hierarchy of binary predicate decisions
- Interpretable model, easy to explain to non-experts
- Popular for classification, also works
- Sensitive to actual features
- Hard to condition well
- Works best with plenty data and few features
- Extension: random forests